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Three-dimensional strain coefficients of resistivity of thin polycrystalline metal films

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Theoretical expressions for the longitudinal and transverse strain coefficients of resistivity in thin polycrystalline metallic films are derived by using a modified form of the three-dimensional conduction model. It has been found that the gauge factors mainly depend on the grain parameter ν and that the thickness variations of these strain coefficients are determined by the grain boundary scattering process, in particular, either an increase or a decrease of gauge factors with thickness may be expected for defined values of ν. Furthermore, a particular value of ν exists for which the film thickness has practically no effect on the gauge factor. Comparison of previously published data on thin metal films shows that some experimental results can be interpreted on the basis of the present model.

1. Introduction

In the past few years several investigators [1–8] have theoretically studied the effects of grain boundaries [1, 8] and film thickness [2–7] on the transverse and/or longitudinal strain coefficient of resistivity of fine-grained metal films. Most of these studies [1–7] have been achieved in the framework of the Mayadas–Shatzkes model [9] or other derived models [4, 5, 10, 11].

However, we have previously shown [12] that the experimental variations of the film resistivity ρ_{F_p} and its temperature coefficient β_{F_p} with the film thickness a can be, for thin sputtered metallic films, satisfactorily interpreted in terms of a new model of conduction denoted the "three-dimensional model" [12, 13]. In this model the effects of grain boundaries and external surface scatterings have been assumed to occur independently of each other and are described by the parameters ν_i and κ [12, 13], respectively, e.g.

$$\nu_i = a_i \cdot l_0^{-1} \cdot \left[\ln \frac{1}{t}\right]^{-1}, \qquad (1)$$

where a_i is the average grain size measured in the i-direction ($i = x, y, z$), t is the transmission coefficient of electrons through grain boundaries which is supposed to be isotropic [13] and l_0 is the background mean free path (mfp) and

$$\kappa = a \cdot l_0^{-1} \cdot \left[\ln \frac{1}{p}\right]^{-1} \qquad (2)$$

where a is the film thickness and p is the fraction of electrons specularly scattered on the external surfaces [14].

In a preceding paper [8] we derived analytical expressions for the strain coefficients of resistivity in the particular case of infinitely thick polycrystalline films (i.e. in the case of totally specular scattering on external surfaces). Thus, in this communication an attempt is made to establish new analytical expressions for the strain coefficient of resistivity in the more general case of partially specular scattering on external surfaces. The calculations are performed as suggested in previous papers [8, 15] in terms of an approximate form of the three-dimensional model [15] which is accurate, as previously shown [8, 15],

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for values of the grain boundary parameter ν greater than 0.4.

2. Theory

It must be pointed out that to undertake the calculation of the strain coefficients of resistivity we have to consider the change in grain size a_i in the three x-, y- and z-directions. To simplify the problem we have modified the expression for the resistivity [15] by considering separately the following contributions to the total film resistivity e.g. [8, 15]:

(a) the contribution $\rho_\perp$ of the grain boundaries perpendicular to the applied electric field E_x (Fig. 1) which is given by [8]

$$\rho_\perp = \rho_0 \{[F(\nu_x)]^{-1} - 1\} \tag{3}$$

with

$$F(\nu_x) = 3\nu_x [\tfrac{1}{2} - \nu_x + \nu_x^2 \ln(1 + \nu_x^{-1})]; \tag{4}$$

(b) the contributions $\rho_\parallel$ of the grain boundaries distributed perpendicular to the y-axis (and parallel to E_x) [8] i.e.

$$\rho_\parallel = \rho_0 \{[G(\nu_y)]^{-1} - 1\} \tag{5}$$

with

$$G(\nu_y) = \tfrac{3}{2}\nu_y [\nu_y - \tfrac{1}{2} + (1 - \nu_y^2) \ln(1 + \nu_y^{-1})]; \tag{6}$$

(c) the contribution ρ^* due to background scattering and to simultaneous electron scattering on the external surfaces and on the grain-boundaries perpendicular to the z-axis which is expressed as [15]

$$\rho^* = \rho_0 [G(\alpha)]^{-1} \tag{6}$$

with

$$\alpha^{-1} = \kappa^{-1} + \nu_z^{-1}. \tag{7}$$

In the above relations ρ_0 refers to the background resistivity.

We have previously shown that an approximate form of the resultant resistivity is then [15]

$$\rho_{F_p}/\rho_0 = M(\nu_x, \nu_y, \alpha) = [F(\nu_x)]^{-1} + [G(\nu_y)]^{-1} + [G(\alpha)]^{-1} - 2. \tag{8}$$

Hence logarithmic differentation of Equation 8 gives, after some rearrangements,

$$\frac{d\rho_{F_p}}{\rho_{F_p}} - \frac{d\rho_0}{\rho_0} = -\frac{1}{M(\nu_x, \nu_y, \alpha)} \left\{ \frac{1}{[F(\nu_x)]^2} \cdot \frac{dF(\nu_x)}{d\nu_x} d\nu_x + \frac{1}{[G(\nu_y)]^2} \cdot \frac{dG(\nu_y)}{d\nu_y} d\nu_y + \frac{1}{[G(\alpha)]^2} \cdot \frac{dG(\alpha)}{d\alpha} \cdot d\alpha \right\}. \tag{9}$$

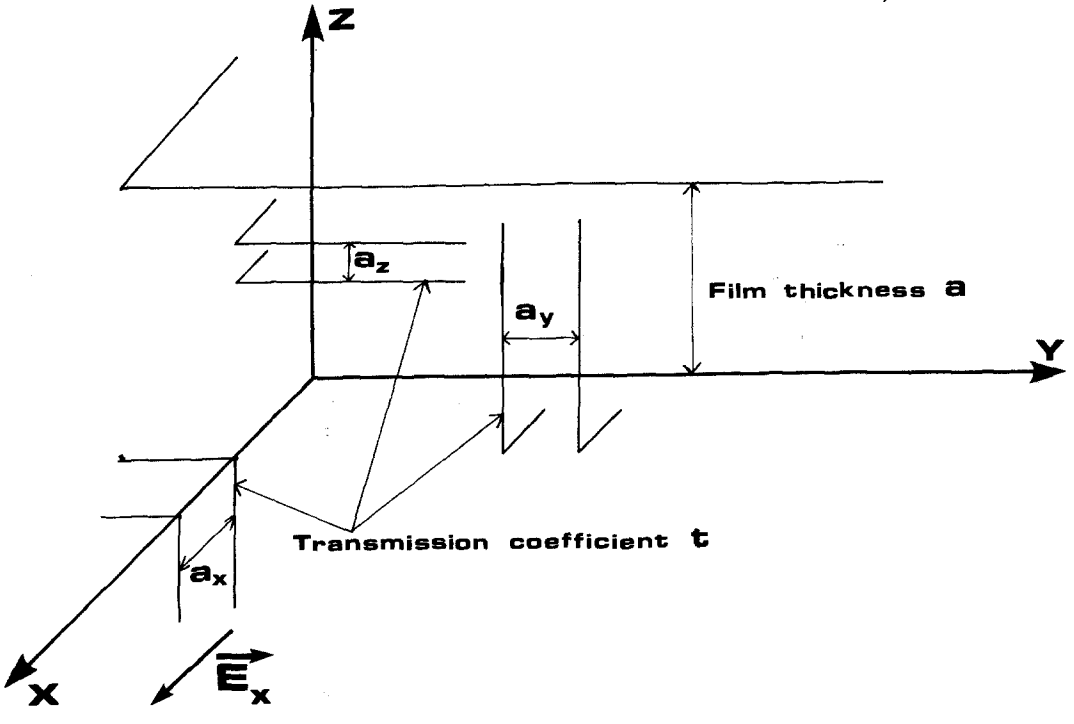

Figure 1 The geometry of the model.

Taking into account that from Equations 1, 2 and 7 we can write

$$\frac{d\nu_i}{\nu_i} = \frac{da_i}{a_i} - \frac{dl_0}{l_0}; \quad i = x, y, z \tag{10}$$

and

$$\frac{d\alpha}{\alpha} = \alpha\left[\frac{1}{\kappa}\left(\frac{da}{a} - \frac{dl_0}{l_0}\right) + \frac{1}{\nu_z}\left(\frac{da_z}{a_z} - \frac{dl_0}{l_0}\right)\right] \tag{11}$$

Introducing Equations 10 and 11 into Equation 9 and defining for convenience the functions

$$f(\nu) = \frac{dF(\nu)}{d\nu} = \frac{3}{2} - 6\nu + 9\nu^2 \ln(1+\nu^{-1}) - \frac{3\nu^2}{1+\nu} \tag{12}$$

and

$$g(\alpha) = \frac{dG(\alpha)}{d\alpha} = \tfrac{3}{2}[3\alpha - \tfrac{3}{2} + (1-3\alpha^2)\ln(1+\alpha^{-1})] \tag{13}$$

which gives, after some mathematical manipulations,

$$\frac{d\rho_{F_p}}{\rho_{F_p}} = \frac{d\rho_0}{\rho_0} + \frac{1}{M(\nu_x, \nu_y, \alpha)}\left(\frac{dl_0}{l_0}\right) \times \left[\frac{\nu_x f(\nu_x)}{F^2(\nu_x)} + \frac{\nu_y g(\nu_y)}{G^2(\nu_y)} + \frac{\alpha g(\alpha)}{G^2(\alpha)}\right] - \frac{1}{M(\nu_x, \nu_y, \alpha)}\left(\frac{da_x}{a_x}\right) \cdot \frac{\nu_x f(\nu_x)}{F^2(\nu_x)} - \frac{1}{M(\nu_x, \nu_y, \alpha)} \cdot \left(\frac{da_y}{a_y}\right) \frac{\nu_y g(\nu_y)}{G^2(\nu_y)} - \frac{1}{M(\nu_x, \nu_y, \alpha)} \cdot \frac{\alpha^2 g(\alpha)}{G^2(\alpha)} \cdot \left[\frac{1}{\kappa}\left(\frac{da}{a}\right) + \frac{1}{\nu_z}\left(\frac{da_z}{a_z}\right)\right]. \tag{14}$$

2.1. The longitudinal strain coefficient of resistivity γ_{F_pL}

It must be kept in mind that when the substrate is bent to produce a longitudinal strain dL/L a transverse strain $dW/W = -\mu_s(dL/L)$ will occur whereas the z-direction (i.e. the thickness direction) is stress free [3, 16]. Under these conditions the well-known elasticity formulae lead to [8]

$$da_x/a_x \approx dL/L \tag{15}$$

$$da_y/a_y \approx dW/W = -\mu_s(dL/L) \tag{16}$$

and

$$da_z/a_z \approx da/a \approx -\mu\frac{(1-\mu_s)}{(1-\mu)}(dL/L) = -\mu'(dL/L), \tag{17}$$

where μ and μ_s are the Poisson's ratios of the film and substrate materials, respectively.

The longitudinal gauge factor γ_{F_pL} of the film is defined as usual [3] as

$$\gamma_{F_pL} = \left(\frac{d\rho_{F_p}}{\rho_{F_p}}\right)(dL/L)^{-1}. \tag{18}$$

In a similar way the bulk value of the longitudinal strain coefficient of resistivity is given as

$$\gamma_{0L} = \left(\frac{d\rho_0}{\rho_0}\right) \cdot (dL/L)^{-1}. \tag{19}$$

Assuming that the film material is isotropic and that the variations of background mean free path l_0 and resistivity ρ_0 with strain ϵ may be entirely attributed to the change in amplitude of the thermal vibrations of atoms the strain coefficient of l_0 and ρ_0 are expressed as

$$d\ln l_0/d\epsilon = -\eta \tag{20}$$

and

$$d\ln \rho_0/d\epsilon = \eta + 1 \tag{21}$$

with

$$\eta = 2g(1-2\mu), \tag{22}$$

where g is Grüneisen's constant [17].

Dividing Equation 14 by dL/L and then introducing Equations 15 to 21, we obtain the final expression of the longitudinal gauge factor γ_{F_pL}

$$\gamma_{F_pL} = (\eta+1) - \eta \cdot [M(\nu_x, \nu_y, \alpha)]^{-1} \cdot [F^*(\nu_x) + G^*(\nu_y) + G^*(\alpha)] + [M(\nu_x, \nu_y, \alpha)]^{-1} \cdot [\mu_s G^*(\nu_y) - F^*(\nu_x) + \mu' G^*(\alpha)] \tag{23}$$

where the functions F^* and G^* are defined by

$$F^*(\nu) = \nu f(\nu) \cdot [F(\nu)]^{-2} \tag{24}$$

and

$$G^*(\alpha) = \alpha g(\alpha) \cdot [G(\alpha)]^{-2}. \tag{25}$$

2.2. The transverse strain coefficient of resistivity γ_{F_pT}

Taking into account the influence of the substrate elasticity on the gauge factor of the film the strain equations become

$$da_x/a_x \approx dL/L = -\mu_s(dW/W) \quad (26)$$

$$da_y/a_y \approx dW/W \quad (27)$$

and

$$da_z/a_z \approx da/a = -\mu'(dW/W) \quad (28)$$

when a transverse strain dW/W is applied to the substrate.

With the preceding assumptions concerning the isotropy of the film material and the change in background mfp and resistivity with applied strain, the calculations carried out in a similar way to that of Section 2.1 yield the final relation

$$\gamma_{F_pT} = (\eta+1) - \eta \cdot [M(\nu_x,\nu_y,\alpha)]^{-1} \cdot [F^*(\nu_x) + G^*(\nu_y) + G^*(\alpha)] + [M(\nu_x,\nu_y,\alpha)]^{-1} \cdot [\mu_s F^*(\nu_x) - G^*(\nu_y) + \mu' G^*(\alpha)]. \quad (29)$$

3. Discussion

Equations 23 and 29 appear to be simple analytical expressions which can easily describe the combined effects of grain boundaries and external scattering processes on the strain coefficient of resistivity of thin polycrystalline metallic films. Before analysing these effects let us show that Equations 23 and 29 satisfy some essential physical requirements, e.g.

(1) When the effects due to grain boundary scattering can be considered as negligible (i.e. $\nu \to \infty$) Equations 23 and 29 tend to the gauge factor expression

$$\gamma_F|_{\text{Cottey}} = (\eta+1)\frac{\kappa_g(\kappa)}{G(\kappa)}(\mu'-\eta) \quad (30)$$

previously deduced [4, 18] from the Cottey [19] mean free path model which only takes into account the contribution to the total resistivity of the external surface scattering. Effectively in the limit of large ν Equation 7 ensures that

$$G(\alpha)|_{\nu\to\infty} \approx G(\kappa)$$

and

$$g(\alpha)|_{\nu\to\infty} \approx g(\kappa)$$

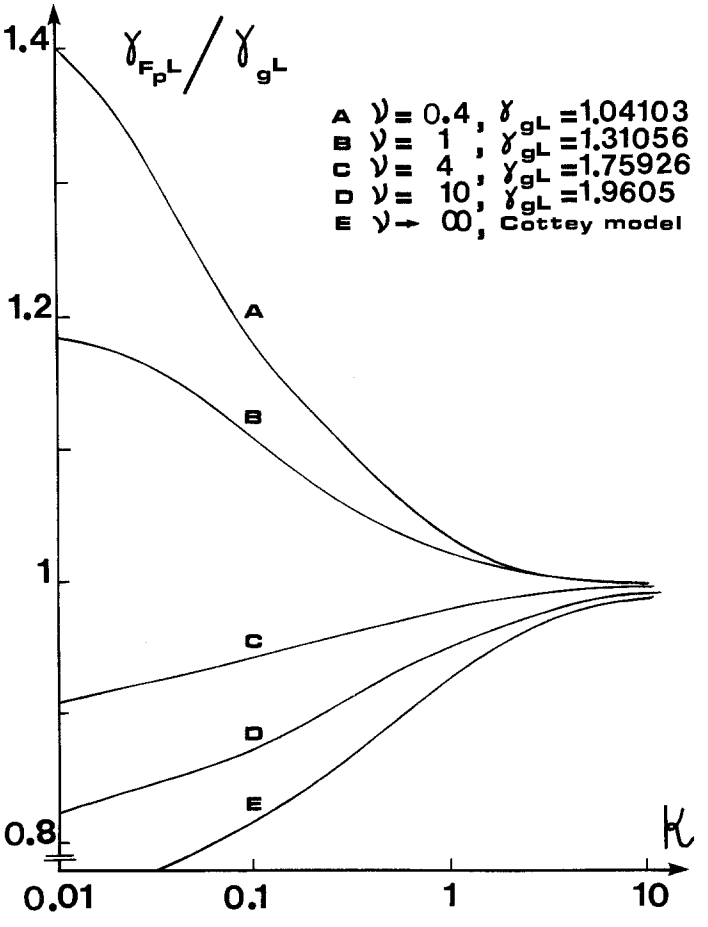

Figure 2 Variation of the gauge factors ratios γ_{FpL}/γ_{gL} with κ parameter for different values of the grain parameter ν.

whereas as previously shown [8] on the one hand the $G(\nu_i)$ and $F(\nu_i)$ tend to unity and on the other hand their derivatives $g(\nu_i)$ and $f(\nu_i)$ approach zero.

(2) When the effect of electron scattering on external surfaces vanishes (i.e. when $\kappa \to \infty$) it easily appears from Equation 7 that the gauge factors γ_{F_pL} and γ_{F_pT} approach the strain coefficients γ_{gL} and γ_{gT} of infinitely thick polycrystalline film e.g. [8]:

$$\gamma_{gL} = (\eta+1) - \eta \frac{F^*(\nu_x)+G^*(\nu_y)+G^*(\nu_z)}{M(\nu_x,\nu_y,\nu_z)} - \frac{F^*(\nu_x)}{M(\nu_x,\nu_y,\nu_z)} + \mu_s \frac{G^*(\nu_y)}{M(\nu_x,\nu_y,\nu_z)} + \mu' \frac{G^*(\nu_z)}{M(\nu_x,\nu_y,\nu_z)} \quad (31)$$

and

$$\gamma_{gT} = (\eta+1) - \eta \frac{F^*(\nu_x)+G^*(\nu_y)+G^*(\nu_z)}{M(\nu_x,\nu_y,\nu_z)} - \frac{G^*(\nu_y)}{M(\nu_x,\nu_y,\nu_z)} + \mu_s \frac{F^*(\nu_x)}{M(\nu_x,\nu_y,\nu_z)} + \mu' \frac{G^*(\nu_z)}{M(\nu_x,\nu_y,\nu_z)} \quad (32)$$

with

$$M(\nu_x,\nu_y,\nu_z) = [F(\nu_x)]^{-1} + [G(\nu_y)]^{-1} + [G(\nu_z)]^{-1} - 2 \quad (33)$$

Figs 2 and 3 represent the thickness dependence of the reduced gauge factors $\gamma_{F_pL}/\gamma_{gL}$ and $\gamma_{F_pT}/\gamma_{gT}$ in the typical case of silver films ($\mu = 0.38$, $\eta = 1.15$ [17]) deposited on a glass substrate ($\mu_s = 0.25$ [20]) assuming as usual [8, 12] that the grain sizes measured in the x-, y- and z-directions take equal values ($\nu_x = \nu_y = \nu_z = \nu$). The choice to present the result in the reduced form γ_{F_p}/γ_g is justified by the fact that we have previously suggested [15] that the departure due to use of an approximate form for the film resistivity is certainly less marked for γ_{F_p}/γ_g against κ plot than for γ_{F_p} against κ plot.

A comparison of Figs 2 and 3 shows quantitative agreement of the observed ν variations with the theoretical predictions of the two limiting cases (i.e. $\nu \to \infty$, $\kappa \to \infty$). In particular it evidently appears that for a large thickness the ratios $\gamma_{F_pL}/\gamma_{gL}$ and $\gamma_{F_pT}/\gamma_{gT}$ take values near unity. In view of this behaviour, previously reported data on metal films [21] can be interpreted on the basis of the present model. Let us particularly examine

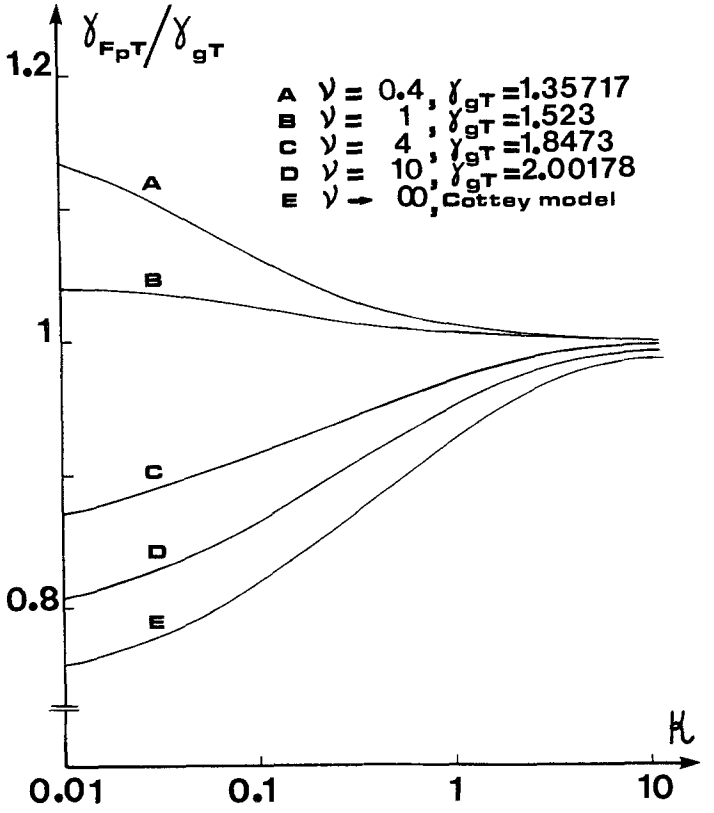

Figure 3 Variation of the gauge factors ratio $\gamma_{F_pT}/\gamma_{gT}$ with κ parameter for different values of the grain parameter ν.

TABLE I Variations of the longitudinal gauge factor γ_{F_pL} of thin silver films for the typical value of the ν parameter: $\nu = 2$ ($\gamma_{gL} = 1.54419$). Note that as the numerical evaluation was performed by means of a pocket calculator the observed very small oscillations are probably due to in accuracies and uncertainties in numerical work.

κ	γ_{F_pL}
0.01	1.5854
0.04	1.5858
0.1	1.5751
0.2	1.5638
1	1.5464
4	1.5440
10	1.5440

the results on evaporated gold film reported by Knight [21]; this author has obtained, by extrapolation, values of the infinitely thick film strain coefficients of resistance which are about half the theoretical bulk values. It is then, in view of the present model, to ascribe this limiting behaviour to the polycrystalline structure of these thick films.

However, Figs 2 and 3 exhibit another interesting feature; it appears that for large values of the ν parameter the gauge factor ratios $\gamma_{F_pL}/\gamma_{gL}$ and $\gamma_{F_pT}/\gamma_{gT}$ increases with increasing values of the κ parameter whereas for small ν these gauge factor ratios decrease with increasing κ. A typical value ν^* of the grain parameter ν exists for which the thickness dependence of the thin polycrystalline gauge factors apparently disappears. In the particular case of silver such behaviour occurs for $\nu^* \approx 2$ (see Table I) indicating that the external surface scattering effect can vanish even when the grain boundaries act as moderately efficient scatterers. It is of interest at this stage to discuss the results of Verma and Juretschke [22] who have measured the strain dependence of the resistivity of thin silver films for film thickness between 30 and 140 nm; the experimental strain dependence of the resistivity does not deviate from that of bulk silver except for some individual films, even at relatively small thicknesses ($a \cdot l_0^{-1} \geqslant 0.59$ with $l_0 \approx 52.3$ nm [23]) suggesting that the absence of any size effect in the gauge factors can be largely governed by grain boundary scattering processes.

4. Conclusion

Analytical expressions of the gauge factors of thin polycrystalline films are derived by using an approximate form of the total film resistivity. The results of the investigation can be summarized as follows:

(a) the role of grain boundaries in determining the thickness dependence of the polycrystalline film gauge factor is predominant;

(b) our studies strongly suggest that the absence of size effect in the gauge factor of thin films can be understood in terms of the present model;

(c) when experimental measurements reveal a decrease (from the bulk values) of the values of the gauge factors γ_{gL} and γ_{gT} of an infinitely thick film these deviations can also be ascribed to dominant scattering mechanisms at grain boundaries.

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